

FAIR Data of Physical and Digital Beamlines

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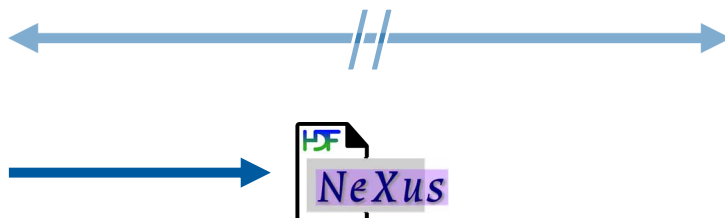
Helmholtz-Zentrum Berlin für Materialien und Energie

Instrument Control (Physical Beamline)



Instrument Life Cycle:

- Planning Phase: Simulation
- Instrument construction
- Commissioning: Verify simulation
- User Operation



Simulation (Digital Beamline)

```
<object name="Slit Horizontal" type="Slit">  
<param id="geometricalShape" value="Cylinder" type="enum"/>  
<param id="totalWidth" enabled="F" type="float" value="14985" unit="mm"/>  
<param id="totalHeight" enabled="F" type="float" value="41750" unit="mm"/>  
<param id="centralBeamStop" type="enum" value="None" type="enum"/>  
<param id="totalWidthStop" type="enum" value="None" type="enum"/>  
<param id="totalHeightStop" type="enum" value="None" type="enum"/>  
<param id="distancePreceding" type="float" value="0" unit="mm"/>  
<param id="azimuthalAngle" type="float" value="0" unit="deg"/>  
<param id="alignmentError" type="float" value="0" unit="mm"/>  
<param id="translationError" type="float" value="0" unit="mm"/>  
<param id="translationError" type="float" value="0" unit="mm"/>  
<param id="rotationError" type="float" value="0" unit="deg"/>  
<param id="rotationError" type="float" value="0" unit="deg"/>  
<param id="rotationError" type="float" value="0" unit="deg"/>  
<param id="worldPosition" type="float" value="0" unit="mm"/>  
<param id="worldXdirection" type="float" value="0" unit="mm"/>  
<param id="worldYdirection" type="float" value="0" unit="mm"/>  
<param id="worldZdirection" type="float" value="0" unit="mm"/>  
</object>
```

Instrument Control (Physical Beamline)

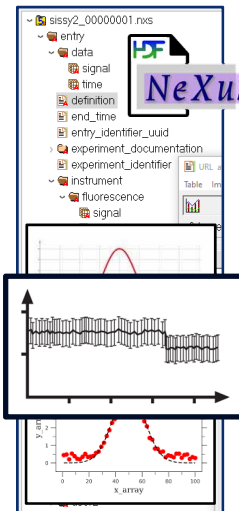


1. Instrument Output
(e.g. motor position)

4. Simulation Feedback
(e.g. resolution)
Correction
(e.g. displacements)

1. Detector Data
(e.g. spectrum)

NeXus File (Data/Metadata)

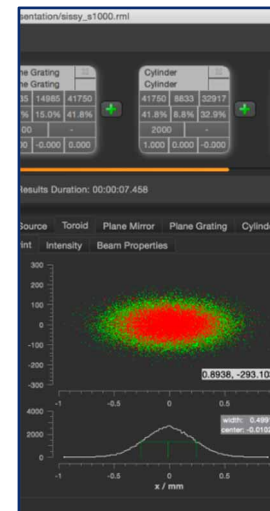


2. Simulation Input
(e.g. geometry)

3. Simulation Output
(e.g. resolution)

5. Machine Learning
(e.g. predictive maintenance)

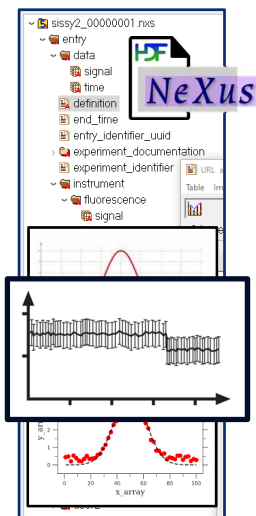
Simulation (Digital Beamline)



Aquarius beamline @ BESSY II, HZB

Repository

NeXus File (Data/Metadata)



Advantages:

- **(Meta)data enrichment:** detailed instrument description increases re-usability
- **Context & Semantics:** relation and nomenclature – where do both worlds match?
- **Interoperability:** same algorithms to access data
- **AI-Ready:** (meta)data is exploitable by AI/ML techniques – simulations from file